Optimising wastewater treatment solutions for the removal of contaminants of emerging concern (CECs): a case study for application in India

Zara Visanji, Seyed M. K. Sadr, Matthew B. Johns, Dragan Savic and Fayyaz A. Memon

ABSTRACT

The aim of this study was to produce optimal wastewater treatment solutions to calculate the removal of different contaminants of emerging concern (CECs) found in developing countries. A new methodology was developed for a decision support tool (WaStewater Decision support OptiMiser, WiSDOM), which focuses on producing treatment solutions suited to treating water for reuse to Indian Water Quality Standards. WiSDOM-CEC analyses the removal of CECs through different treatment solutions and was also used to evaluate the performance of each treatment train solution in terms of the removal of conventional pollutants using multi-objective optimisation and multi-criteria decision analysis. Information was collected on different CECs across different regions of India, and the removal of 18 different CECs through 42 wastewater treatment unit processes for five different regions of India was analysed. Comparisons between similar categories of CECs, such as non-steroidal anti-inflammatory, showed that emerging contaminants all react differently with individual treatment options. For example, the removal of ibuprofen (IBP) and naproxen (NPX) varied from >80% and 0%, respectively, for a solution in Karnataka involving sedimentation, submerged aerated filter, ultrafiltration and nanofiltration. In Tamil Nadu, results ranged from 36.8% to 72% for diclofenac, 10.7% to 66.5% for IBP, and 0% for NPX.

Key words | contaminants of emerging concern, decision support tool, India, water quality, WiSDoM

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INTRODUCTION

Contaminants of emerging concern (CECs) have been detected since 1965 (Stumm-Zollinger & Fair 1965), when the first steroid hormones were revealed in the aquatic environment. Since this time, there have been advances in technology leading to the improved detection and analysis of increased quantities of CECs at levels ranging from microgram per litre (μg/L) to nanogram per litre (ng/L) using a range of techniques (Calvo-Flores *et al.* 2018). CECs are frequently defined as naturally occurring, synthetic or anthropogenic chemicals/substances, which are not regularly monitored (Visanji *et al.* 2018). These substances also have a negative impact on the environment and human health; however, further toxicological studies are required to determine the full toxicity implications of these substances. The main categories of CECs commonly reported in the literature are: (i) pharmaceuticals, (ii) personal care products, and (iii) endocrine disruptors (Fischer *et al.* 2017; Montes-Grajales *et al.* 2017; Tran *et al.* 2018). More recently, an increasing number of publications have also included other categories such as steroid hormones, surfactants (i.e., nonylphenol and octylphenol), perfluorinated compounds (i.e., perfluorooctane sulfonate and perfluorooctanesulfonic acid), flame retardants (i.e., polybrominated biphenyl ethers), industrial additives and

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agents, illicit drugs, UV filters, and artificial sweeteners (Baalbaki *et al.* 2017).

The dominant pathway that allows CECs to enter the aquatic environment is via the effluent of wastewater treatment plants, with other pathways including veterinary locations and surface runoff from agricultural areas (Lapworth *et al.* 2012). Human bodies are unable to fully metabolise pharmaceutical compounds causing CECs to be excreted via urine and faeces (Anumol *et al.* 2016). Unfortunately, wastewater treatment plants were not originally designed to remove these compounds (Tran *et al.* 2018). Therefore, CECs can pass through as parent compounds or metabolites (a transformed product) and continuously enter the environment. In some locations, water is abstracted downstream of wastewater treatment plants and processed through a water treatment plant for drinking water. These water treatment plants are also unable to efficiently remove CECs allowing them to contaminate drinking water. Therefore, it is important that the removal of CECs through existing and new technologies is thoroughly explored. The design of effective treatment solutions requires such analysis to further reduce the concentration circulating through the environment and humans.

Environmental regulations for CECs are limited to developed countries, with only a few monitoring processes put in place for some developing countries. Unlike developing countries, the European Union (EU) has implemented a watch list (EU 2015/495) on priority substances classed as CECs (European Union 2015). The EU has also introduced and applied legislations such the Regulation of Registration, Authorisation and Restriction of Chemicals (REACH), which focuses on monitoring chemical substances when manufactured or imported (REACH 2016). Research programmes in the UK have also been carried out to better understand and monitor the problem at hand, including the Chemicals Investigation Programme (ALS Environmental 2015) and the National Implementation Plan (DEFRA 2017). The USA have produced the Contaminants Candidate List which focuses on unregulated drinking water contaminants (US EPA 2016).

Developing countries such as South Africa, Brazil, China, and India currently have no official legislation surrounding CECs; however, an increase in publications and research has allowed for a clearer indication of the problem in these countries. In Brazil, around 50% of wastewater does not pass through a treatment facility (Machado *et al.* 2016) further reducing the chances of CECs being removed from the effluent due to less treatment occurring in the first place. In the past 19 years in Brazil, levels of CECs have reached the following concentrations: 6,806 ng/L for hormones, 20,960 ng/L for acetyl salicylic acid concentrations in rivers, 14,955 ng/L for caffeine, up to 785 ng/L for diclofenac (DCF), 5,896 ng/L for cocaine and for paracetamol concentrations have exceeded 30,000 ng/L (Starling *et al.* 2018).

India is currently one of the top pharmaceutical emerging markets in the world, and one of the largest global providers of medicines (drugs) accounting for 20% of global exports. Proper wastewater management techniques do not exist in India, and conventional treatment plants are inefficient at the complete removal of CECs, with sewage treatment plants discharging their effluent to rivers. The Bureau of Indian Standards is not currently addressing CECs and not all regions of India have carried out investigations on CECs (Philip *et al.* 2018); therefore, it has become essential for the creation of baseline data to act as a framework for any future research or regulatory initiatives. The latest reports show that sewage generated from towns and cities in India is not being fully treated, with only 11,787 million litres per day (MLD) receiving treatment from 38,255 MLD (Philip *et al.* 2018). The concentration of certain CECs such as antibiotics are seen to be 40 times higher in Indian wastewater treatment plants than other countries (Balakrishna *et al.* 2017), suggesting that the effluent from wastewater treatment plants is contaminated with CECs even though treatment has occurred.

Balakrishna *et al.* (2017) explored the occurrence of pharmaceuticals and personal care products in the influent and effluent of wastewater treatment plants in India and detected 73 different CECs. High concentrations of artificial sweeteners were seen in both the influent and the effluent ranging from 143,000 (ng/L) to 389,000 ng/L and 6,020 to 379,000 ng/L, respectively. Recorded caffeine concentrations were also high ranging from 19 ng/L to 102,840 ng/L (Balakrishna *et al.* 2017), whereas levels in the European Union were seen to reach 3,000 ng/L (Loos *et al.* 2012). A more recent review carried out by Philip *et al.* (2018) documents the extensive occurrence of CECs throughout the different regions of India with the detection of 166 different CECs belonging to 36 main categories. The highest recorded concentration in surface waters of India is noted as ciprofloxacin, reaching 14,000,000 ng/L. In Northern India, lower levels of antibiotics were found in rivers during the monsoon season; however, a study by Mohapatra *et al.* (2016) found high levels of antibiotics during the monsoon season in comparison to winter and summer. High levels of antibiotics were also recorded during the monsoon season in the South of India, along with pharmaceuticals due to an increased use during this time (Philip *et al.* 2018). Caffeine values reaching <150,000 ng/L were seen during summer months, with concentrations in winter reaching <40,000 ng/L (Mohapatra *et al.* 2016).

With the above understanding of the problem of CECs and the need for proper wastewater management in less developed countries, this paper aims to produce optimal wastewater treatment solutions for developing countries. The selection of wastewater treatment solutions involves intricate decision-making, incorporating all elements of treatment (from preliminary options through tertiary treatment and disinfection), to ensure a suitable relationship exists between the biological, physical, and chemical processes needed to treat wastewater to the required levels (Poch *et al.* 2014). Sadr *et al.* (2018) proposes that for developing countries, the selection process becomes even more complex as additional considerations are needed due to a variety of socio-economic and environmental factors that exist in these countries. WiSDOM (WaStewater Decision support OptiMiser), which is a decision support tool, was created to include these additional parameters (capital, operational and maintenance costs, energy consumption, chemical requirement, land requirement, and reliability). A range of decision objectives and criteria have been incorporated into the tool as a process of formulating wastewater treatment solutions (Sadr *et al.* 2018). This will allow stakeholders and decision makers to implement sufficient wastewater treatment solutions for proper wastewater management to treat wastewater to desirable levels. This paper describes the development and application of a new methodology WiSDOM-CEC, which was encapsulated as a software programme (as an add-in for a stand-alone user-friendly decision support tool – WiSDOM) used to calculate the removal rates of CECs during different wastewater treatment processes. India is used as a case study, with scenarios developed to demonstrate WiSDOM-CEC's application when combined with an existing decision support tool. The scenarios focused on five different regions of India (North, South Western, South, North Eastern, and Central) to analyse the removal efficiencies for antibiotics, nonsteroidal anti-inflammatory drugs, and other categories of CECs (hormones, stimulants, personal care products, and insect repellents).

METHODS

The main aim of this study was to analyse the performance of different treatment unit trains to determine their efficiency at removing CECs. This section describes the methodology for WiSDOM-CEC employed to analyse the removal of CECs from different treatment processes generated in India, using an existing decision support tool, WiSDOM. The tool currently does not incorporate the removal of CECs; therefore, a new software programme (Excel Spreadsheet Programme (ESP)) was designed to work alongside WiSDOM. The ESP calculates the removal of CECs once treatment solutions were populated through WiSDOM depending on specific user requirements and objectives. The methodology for the ESP was originally developed to calculate the removal of 39 CECs for 42 WiSDOM-generated wastewater treatment trains (Visanji *et al.* 2018). However, this paper focuses on the removal of CECs commonly recorded within India. Due to the limited published data on the removal of CECs in India, removal rates for different treatment unit processes were taken from publicly available sources to ensure a complete dataset.

WiSDOM: a decision support tool

WiSDOM is a user-friendly tool designed to aid in the formulation of wastewater treatment trains for the removal of conventional pollutants in different contexts. WiSDOM evaluates the performance of each solution with respect to different objectives. The tool also calculates the removal of the following conventional pollutants by each generated treatment train: (i) chemical oxygen demand (COD), (ii) biochemical oxygen demand (BOD), (iii) total suspended solids, (iv) total nitrogen (TN), (v) total phosphorus, (vi) faecal coliform (FC), (vii) turbidity, (viii) intestinal nematode eggs (INEs), and (ix) *Escherichia coli*.

WiSDOM was chosen to generate treatment solutions as it determines the optimal treatment options considering sustainability indicators and ensuring that the removal of conventional pollutants meets the different water reuse standards in India (Table 1). At the core of the software is a technology library that contains detailed information on a wide range of wastewater treatment processes applicable within the context of India (Sadr *et al.* 2018). The tool uses the technology library and a multi-objective optimisation (MOO) algorithm to generate optimal wastewater treatment trains which are then processed by a multi-criteria decision analysis (MCDA) technique to narrow down the resultant non-dominated solution set. The user is given two choices of MOO algorithm; the Non-Dominated Sorting Genetic Algorithm II (NSGA-II) (Deb *et al.* 2002) and the Omni-optimizer (Omni) (Deb & Tiwari 2008). The two algorithms have shown to handle the vagaries of practical optimisation problems well and prove suited to the formulation of wastewater treatment trains. The user has full control over the formulation of the problem; from defining which objectives are being considered for optimisation to the hydraulic, water quality, and design constraints.

The available optimisation objectives are as follows: (1) Capital Expenditure (CAPEX), (2) Operational and Maintenance Expenditure (OPEX), (3) energy consumption, (4) sludge production, (5) land requirement, and (6) labour requirement, all of which are minimised by the optimisation process. Following the MOO, compromise programming (CP), a MCDA technique is used to assess the solutions according to user-defined weighting of various criteria spanning a range of design aspects including technical, environmental, and social and economic considerations (Sadr *et al.* 2018). CP calculates the distance each solution is from the theoretical ideal. The solutions are then ranked according to this 'comprise distance' and displayed to the user. The ESP (described further below) was created as an add-in to WiSDOM, using the results from the tool depending on the scenario or the context defined by the user. For the purpose of this study, the MOO objectives, parameters, and MCDA criteria weight settings were set to their relevant default settings (Sadr *et al.* 2018). For each set of data, NSGA-II is applied with a termination criterion of 12,000 fitness evaluations, population size of 75, a cross-over rate of 0.85 and a mutation rate of 0.15. These parameter values were obtained through experimentation to ensure near optimal algorithm performance on the problems in question (Sadr *et al.* 2018).

It should be noted that although separate regions of India were chosen for the tool's application, assumptions were made regarding the input factors (found in Table S2 in the Supplementary Information) to ensure that the results focused on the removal of CECs:

(1) For the scenario, the genetic algorithm objectives, parameters, and MCDA criteria weight were set to either urban or rural settings. This was dependent on where most of the population lived. For example, in Delhi, 97.5% of the population live in urban regions, whereas in Karnataka 61.3% live in rural areas (Census 2011). Therefore, Delhi would be set to the urban default settings and Karnataka as rural.

Table 1 | Indian water quality standards for reuse application (Sadr *et al.* 2017)

Contaminants	Toilet flushing	Vehicle exterior washing	Horticulture	Non-edible crops	Edible crops — raw	Edible crops — cooked
COD (mg/l)	16	16	16	30	16	30
BOD (mg/l)	10	10	10	20	10	20
Suspended solids (mg/l)	40	35	40	30	25	30
TN (mg/l)	10	10	10	10	10	10
Phosphorus (mg/l)	1	1	2	5	2	5
FC (no./100 ml)	0	0	0	230	0	0
Turbidity (NTU)	<2	<2	<2	<2	<2	<2
INEs (no./100 ml)	<2	<2	<2	<1	<1	<1

(2) The treatment train solution was set to include the following number of each unit process: 1 × preliminary treatment, 1 × primary treatment, 2 × secondary treatment, 2 × tertiary treatment and 1 × disinfection.
(3) Due to limited data available, the influent concentrations (found in Table S1 – 1, S1 – 2 and S1 – 3, Supplementary Information) for the wastewater influent conventional contaminants were all set to WiSDOM's default values.
(4) Certain unit processes (listed below under the ESP) were removed from WiSDOM as a potential solution due to the lack of data on CECs, therefore, eliminating them as a treatment train solution.

It is important to note that WiSDOM is used as a wastewater reuse tool, whereby treatment solutions that are provided are aimed at treating the water to a higher water quality standard than regular wastewater treatment plants. For example, urban areas were set to be reused for toilet flushing, whereas rural areas had an intended reuse application for non-edible crops, therefore resulting in the level of treatment being higher than if the end use was aimed at discharge into a river. Incorporating a water reuse function allows the treatment trains to provide a higher water quality as the effluent. However, in some cases, the unit processes selected by the tool, such as reverse osmosis, are not always the most efficient process to treat CECs, especially in the conditions of rural India, where some of the suitable treatment options of advanced oxidation are not a practical option for the surrounding conditions.

More details on WiSDOM can be found in Sadr *et al.* (2018). (All work with WiSDOM has been built upon original research carried out by Joksimovic *et al.* (2008, 2006).)

New methodology: WiSDOM-CEC

WiSDOM-CEC was formed from a new methodology encapsulated as a software programme, the ESP. The ESP used to determine the removal of CECs from different treatment unit processes, previously generated in WiSDOM, and was created from three different separate worksheets. Removal efficiencies were researched for each treatment option taken from the WiSDOM tool. Three worksheets were combined using functions and formulas to allow for a user-friendly software programme; this is explained further in Visanji *et al.* (2018). A database was created containing over 500 recorded CECs with data present from many countries. The database was used to gather information on 39 CECs; however, only 17 were chosen for the final study. The database included abbreviations of CECs, their chemical abstract service number, and recorded minimum and maximum concentrations from surface water, groundwater, untreated wastewater, drinking water, and treated wastewater.

To produce WiSDOM-CEC, different components and datasets were pulled from other tables/spreadsheets and populated into a singular user-friendly ESP. The names of the CECs from Spreadsheet B along with minimum and maximum initial concentration values (ng/L) were inputted into the first four columns. The top three rows consisted of the stage of treatment, including drop-down options allowing the user to select the ID number for a unit process (from Spreadsheet A). The ESP matches the treatment unit processes used within WiSDOM; therefore, the ESP contained the same stages and unit processes' ID numbers. The drop-down option for the unit processes was taken from Spreadsheet A, as the ID number is changed the treatment changes to the name corresponding process from Spreadsheet C. This allows the ESP to take the relevant removal percentage from Spreadsheet C of each individual CEC, depending on the treatment process chosen. The main section of the ESP involved an equation (Equation (1)), which calculated the removal of CECs throughout different unit processes which have been selected. Equation (1) was used across the ESP which takes the removal rates associated with a unit process from Spreadsheet C and calculates the new concentration (ng/L) after that treatment unit. If the concentration after a treatment stage reaches the desired level (defined by the tool user), then the words 'No Further Treatment' will appear, showing the end user where the CEC was fully removed. The inbuilt 'IF' function in Excel is used to change the information regarding removal rates (from Spreadsheet C), depending on the unit process ID number selected by the user within the drop-down options on the ESP.

$$Y_m = I_m \times \prod_{k=1}^{S} (1 - R_{m,u,k})$$

where m is the contaminant ID; k the stage of treatment; S the maximum number of stages considered in the proposed treatment train; I_m the influent quality with respect to concentration (ng/L) of m; Y_m the effluent quality with respect to concentration (ng/L) of m and $R_{m,u,k}$ the contaminant removal rate (%) of the unit process u in treatment stage k.

An example demonstrating the components of the ESP and Equation (1) are demonstrated below for a treatment train with four stages (see Equations (2) and (3)) for removal of DCF. As shown in Figure 1, in the first stage, a grit chamber process is selected (used as a preliminary/primary treatment). This process, however, does not remove any of the DCF in the wastewater. A membrane bioreactor (MBR) was applied in the second stage; this unit process can remove around 40% of DCF (Luo *et al.* 2014). The MBR is followed by a nanofiltration (NF) and an ultraviolet (UV) process with DCF removal rates of 60% and 40%, respectively. The initial concentration of DCF was 9,520 ng/L and after going through all the four stages is 1,370 ng/L, which means that the total DCF removal efficiency of this treatment train is 85%.

$$Y_{\mathrm{DCF}} = I_m \times \prod_{k=1}^{S=4} 1 - R_{m,u,k}$$

$$Y_{\mathrm{DCF}} = 9,520\,\mathrm{ng/L} \times [(1-0)\times(1-0.4)\times(1-0.6)\times(1-0.4)]$$
$$\rightarrow Y_{\mathrm{m}} = 1,370\,\mathrm{ng/L}$$

WiSDOM-CEC considered a range of assumptions to allow for a more complete dataset of removal rates for different treatment processes. Previous research (Luo *et al.* 2014; Petrie *et al.* 2015; Tran *et al.* 2018) focuses on the overall removal rate of CECs through different treatment trains and does not focus on individual treatment unit processes. To date and to the best of the authors' knowledge, information surrounding the breakdown of the removal efficiencies within the effluent at different stages of treatment is unavailable. In addition, insufficient data exist for each emerging contaminant and each unit process which has been chosen. Consequently, where no data were found for an individual treatment process, a removal rate of 0% was inputted into the cells to produce a complete dataset, allowing for the calculations within the ESP to effectively run. The treatment options set to 0% removal were: bar screen, grit chamber, coarse screen, fine screen, Actiflo, enhanced biological phosphorus removal, P-precipitation and soil aquifer treatment, which are all within the categories of preliminary or primary treatment.

The results from WiSDOM-CEC are displayed in tabular and graphical format. A bar chart of the CECs final concentration in the effluent for both minimum and maximum removal rates is displayed. Results are shown for the final concentration after each treatment train and at the end of each individual unit process. For this study, maximum influent concentrations are used, and graphs are displayed for both minimum removal and maximum removal. This is due to the ESP having two removal settings that allow for

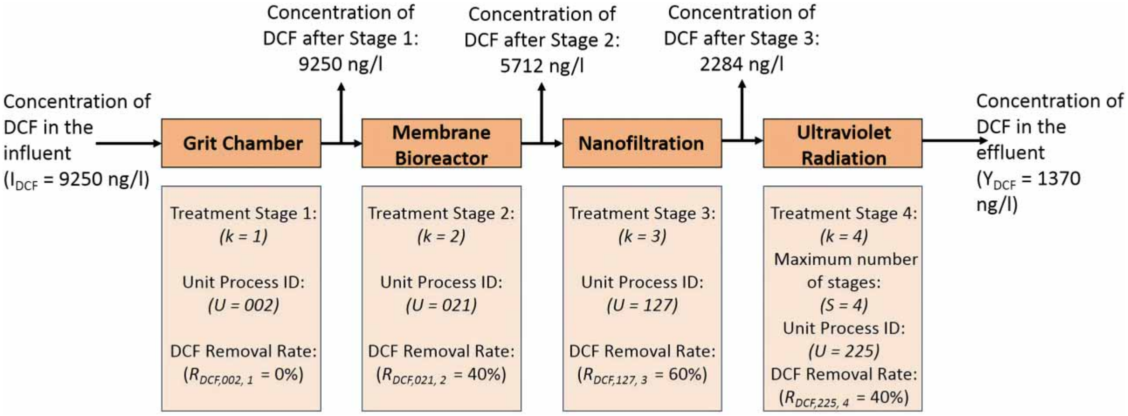

Figure 1 | A treatment train schematic showing the input concentration and output concentration of Diclofenac. The percentage values represent the removal rates for the unit process which has been used.

different removals to be calculated as both data on minimum and maximum removal rates are present. For example, Diazinon is able to be removed from 75% to 100% when advanced oxidation is used (Samadi *et al.* 2007); therefore, the results would show the removal for both these rates.

Scenario development: India

For this study, an initial review was carried out on existing literature published within India, to find the most commonly recorded CECs (see Supplementary Information, Table S1). Following these, 17 CECs that were present within the ESP were chosen to further explore their removal efficiencies within wastewater treatment plants. The CECs chosen in the study can be seen in Table 2 and consisted of pharmaceuticals, a hormone, a stimulant, personal care products, and an insect repellent.

The scenario used to test the application of the tool and ESP looked at investigating the different regions of India and wastewater treatment technologies that would be suitable for removing the concentrations of CECs found in the North, North East, South, South West, and Central India. This was done by focusing on the removal efficiencies for CECs with similar properties categorised by different drug classes.

a. To compare and find optimal treatment solutions for the removal of different antibiotic classes (penicillin, fluoroquinolone, macrolide, quinolone, sulphonamides and trimethoprim).

Table 2 | Concentrations of CECs recorded in different regions of India (the data in this table are adapted from Table S2 and can be found in the Supplementary Information, including all references)

Region	**North**		**South Western**	**South**	**North Eastern**	**Central**
Location	**Utter Pradesh**	**Delhi**	**Karnataka**	**Tamil Nadu**	**Bihar**	**Nagpur**
Emerging contaminant	Concentration (ng/L)					
Pharmaceuticals						
Ampicillin	–	104.2	–	–	–	–
Atenolol	–	–	192–2,900	110–2,440	1.3–1,010	–
Carbamazepine	4.49–650	–	1–726	75–840	82–270	–
Ciprofloxacin	4.8–16	20.06	–	–	7–28.8	12,900
Diclofenac	1.68–360	–	15–412	170–540	1.41–2.55	–
Erythromycin	–	–	–	12	–	–
Ibuprofen	1,430–2,380	–	17–4,460	2,140	686–1,130	–
Naproxen	1.67–120	–	14–235	23–510	2.4–2.62	–
Ofloxacin	–	–	–	212	–	–
Sulfamethoxazole	10.7–27.5	–	5–2,260	3–480	11–17.5	–
Triclosan	5.4	–	892–2,440	2,500	145–450	4,890
Trimethoprim	210–4,010	–	21–180	3–240	33–90	–
Hormones						
Estrone	–	–	10–124	–	–	–
Stimulants						
Caffeine	17.5–40	–	14–61,000	41,000–220,000	16–743	102,840
Personal care products						
Benzophenone	–	–	–	–	–	3,960
Bisphenol A	–	–	59–299	–	–	–
Insect repellent						
N,*N*-diethyl-meta-toluamide	6.4–22.3	–	15–388	9.1–50	4–4.5	–

b. To compare and find optimal treatment solutions for the removal of nonsteroidal anti-inflammatory drugs (NSAIDs) (DCF, ibuprofen (IBP), and naproxen (NPX)).
c. To compare and find optimal treatment solutions for the removal of the other categories of CECs (hormones, stimulants, personal care products and insect repellents).

RESULTS AND DISCUSSION

Results from the optimisation (in WiSDOM) of the objectives such as CAPEX, OPEX, and land are displayed as a radar plot where the higher the point on the axis the greater the performance of the solution. However, results for the removal of conventional pollutants work in a reverse effect where the higher the point on the axis the worse the solution has performed, as this graph compares the performance of each solution in regard to contaminant removal. However, it should be noted that all treatment solutions have met the required Indian Water Quality Standards and the performance noted is a comparison to the other solutions. The treatment trains outputted in the WiSDOM tool were then processed through the ESP to determine their capability of removing CECs. Data from the ESP showing the removal of CECs are presented as bar charts. The below results display the solutions across different regions in India, with sections also focusing on the removal across the categories of CECs (antibiotics, NSAIDs, hormones, stimulants, personal care products, and insect repellents). Results are displayed for Uttar Pradesh, Delhi, Karnataka, and Tamil Nadu in the main text, with the results for Bihar and Nagpur presented in S3 in the Supplementary Information.

Uttar Pradesh

Results for Uttar Pradesh from the WiSDOM tool populated six optimised treatment solutions which fit the original constraints entered into the tool (found in Table S1, Supplementary Information). Table 3 displays the treatment train selected for each solution generated.

Table 3 | Wastewater treatment solutions taken from the WiSDOM tool for Uttar Pradesh

Solution number	Treatment train
1	Constructed wetlands → advanced oxidation – UV/O_3
2	Constructed wetlands → advanced oxidation – UV/H_2O_2
3	Constructed wetlands polishing → chlorine dioxide
4	Constructed wetlands polishing → ultrafiltration
5	Coarse screen → fine screen → sedimentation → trickling filter + secondary sedimentation → ultrafiltration
6	Grit chamber → dissolved air flotation (DAF) → conventional activated sludge process (CASP) + secondary sedimentation → ultrafiltration

Solution (S) 6 outperformed the other solutions at removing conventional pollutants, and in regard to the sustainability indicators performed poorly for land, and performed highly for CAPEX and OPEX (Figure 2). S5 performed well for the conventional pollutants and like S6 performed well for CAPEX and OPEX. S4 performed in the middle for conventional pollutants, and still had low rates in comparison to S1, S2, and S3. S3 performed the worst in regard to CAPEX and OPEX, and ranked second best in regard to land requirements. S2 had a similar pattern to S3, whereas S4 performed highly in all the categories. Regarding the MOO objectives, the solutions that met most of the requirements were S4 if the focus was on sustainability indicators, or S6 if the focus was on removal of conventional pollutants.

The use of constructed wetlands (CWs) with advanced oxidation techniques was able to remove most of the CECs apart from Ciprofloxacin (CIP) which was left with a 0% removal. S1 was able to remove IBP and Sulfamethoxazole (SMZ) to 100%, and DCF, Triclosan (TCS), caffeine (CAF), and N,N-Diethyl-m-toluamide (DEET) to greater than 90% removal. The use of advanced oxidation H_2O_2 in S2 allowed the removal of DCF to increase from 95% in S1 to 100% removal in S2. However, no other CECs were affected by the change in advanced oxidation. When chlorine dioxide was incorporated in S3, the removal of TCS dropped to 0% removal, showing that there is no impact from CWs. The removal rates of CBZ, CAF, and DEET also dropped to 40%, 59% and 55%, suggesting that a higher quantity of removal was processed at advanced oxidation. S4 showed the lowest removal rates, with four of the CECs having a 0% removal

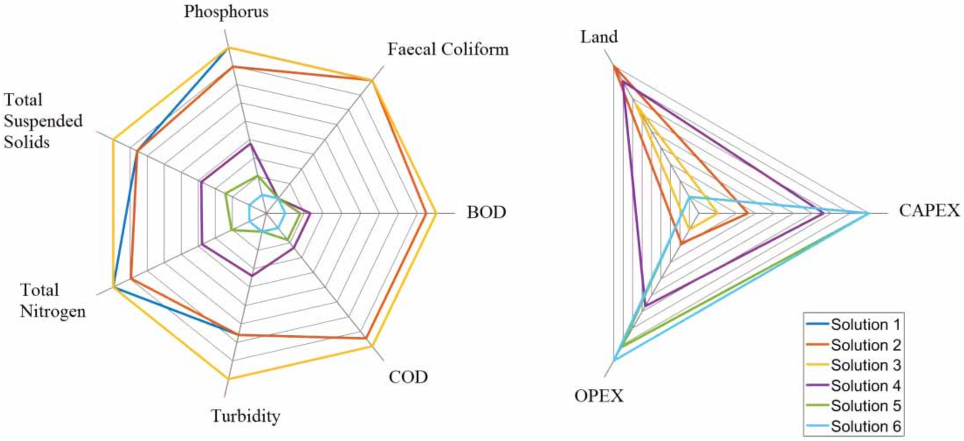

Figure 2 | Performance results from WiSDOM. (Left) Radar plot from the MOO optimisation for the results for the performance of the removal of conventional pollutants for all solutions. The higher the point on the axis the worse the solution has performed. (Right) Radar plot from WiSDOM from the MOO optimisation for the results for the performance of different sustainability indicator objectives (Land, OPEX, and CAPEX). The higher the point on the axis the better the solution has performed.

(Figure 3). S5 was unable to remove NPX and minimal removal rates dropped to 0%; however, TCS and CIP were removed to 97% and 83%, respectively. Lastly, S6 was the only solution able to remove all the CECs; however, the maximum removal rates which reached 100% removal for CIP, DCF, IBP, and SMZ in S3 dropped to 92.3%, 82.5%, 66.5%, and 60%, respectively. Overall, the best solution to remove the majority of the CECs would be S2 or S6; however, S6 was also able to outperform S2 when removing conventional pollutants.

Delhi

Results for Delhi from the WiSDOM tool populated six optimised treatment solutions which fit the original constraints entered into the tool (found in Table S1, Supplementary Information). Table 4 displays the treatment train selected for each solution generated.

Solution (S) 4 performed poorly compared to the other solutions in regard to the sustainability indicators and objectives inputted into WiSDOM (Figure 4), and also performed

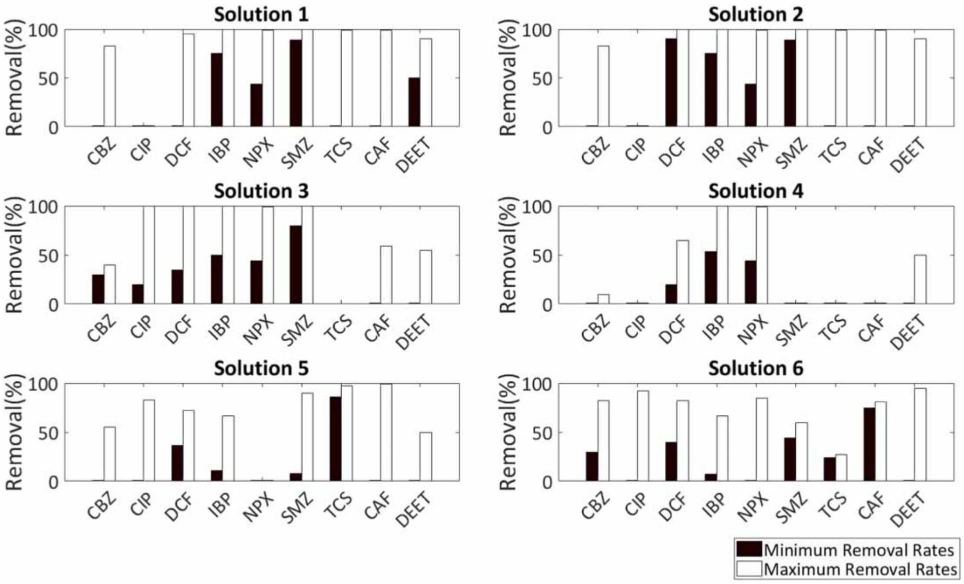

Figure 3 | Percentage of CECs removed from the different treatment solutions produced from WiSDOM-CEC for Uttar Pradesh.

Table 4 | Wastewater treatment solutions taken from the WiSDOM tool for Delhi

Solution number	Treatment train
1	Bar screen → fine screen → CASP → powdered activated carbon (PAC) → reverse osmosis
2	Bar screen → fine screen → CASP → microfiltration → reverse osmosis
3	Sedimentation → trickling filter + secondary sedimentation → PAC → reverse osmosis
4	Bar screen → fine screen → CASP → ultrafiltration
5	Grit chamber → dissolved air flotation (DAF) →trickling filter + secondary sedimentation → PAC → nanofiltration
6	Grit chamber → sedimentation → CASP → microfiltration → nanofiltration

the worst in regard to the removal of conventional pollutants compared to the other solutions. S3 outperformed all solutions when looking at the removal of conventional pollutants (Figure 4) and performed highly in regard to CAPEX and OPEX but low in regard to land requirements. S6 was the best solution at meeting land requirements but had similar results to S5 in regard to conventional pollutant removal. S5 was the second worst solution at both MOO objectives (Figure 4). The best solution to remove conventional pollutants was S3, and this solution also was suited to meeting the requirements for CAPEX and OPEX, although it performed poorly in regard to land requirements. Therefore, this would be the best solution if land requirements were not a preference.

When using the above solutions to determine the best solution for the removal of CECs, it is interesting to see similar results due to the unit processes used. S5 was unable to remove either Ampicillin (AMP) or CIP through this treatment train, showing that the use of either a grit chamber, Dissolved Air Flotation (DAF), trickling filter, PAC or NF does not contribute to the removal of these contaminants. S6 was able to remove CIP by 98.7% at maximum removal, whereas S1, S2, and S4 were only able to remove 92.3%, and S3 only reached 83% removal (Figure 5). For all solutions when the ESP's minimal removal rates were considered, there was no removal of CIP leading to a 0% removal rate. For AMP, only S1, S2, and S3 were able to remove this contaminant to 25.9 ng/L at minimal removal rates causing a 75.1% removal, and to 1.97 ng/L when maximum removal rates were considered leading to a 98.1% removal of this contaminant. The best treatment option for the removal of these two CECs would be S1, S2, and S3 as these were able to remove both CECs. However, from Figure 2, we know that S3 was the solution that outperformed the others in regard to the constraints set for Delhi.

Karnataka

Results for Karnataka from the WiSDOM tool populated six optimised treatment solutions which fit the original constraints entered into the tool (found in Table S1, Supplementary Information). Table 5 displays the treatment train selected for each solution generated.

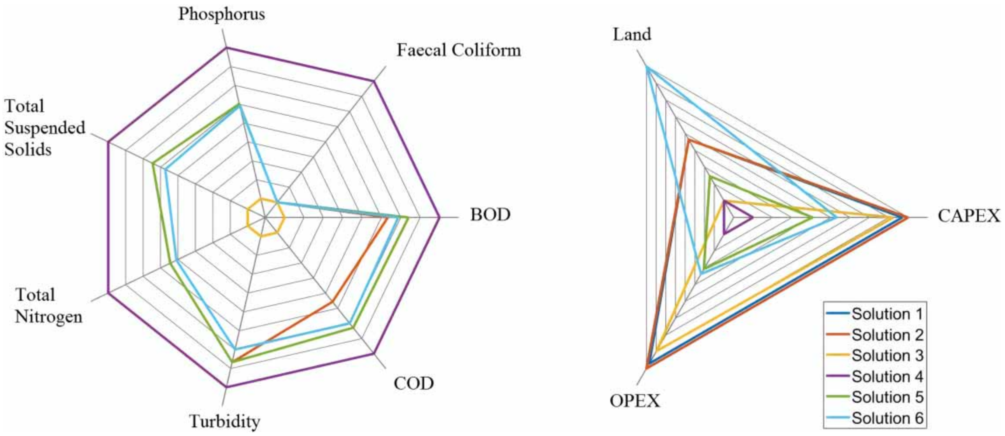

Figure 4 | Performance results from WiSDOM. (Left) Radar plot from the MOO optimisation for the results for the performance of the removal of conventional pollutants for all solutions. The higher the point on the axis the worse the solution has performed. (Right) Radar plot from WiSDOM from the MOO optimisation for the results for the performance of different sustainability indicator objectives (Land, OPEX, and CAPEX). The higher the point on the axis the better the solution has performed.

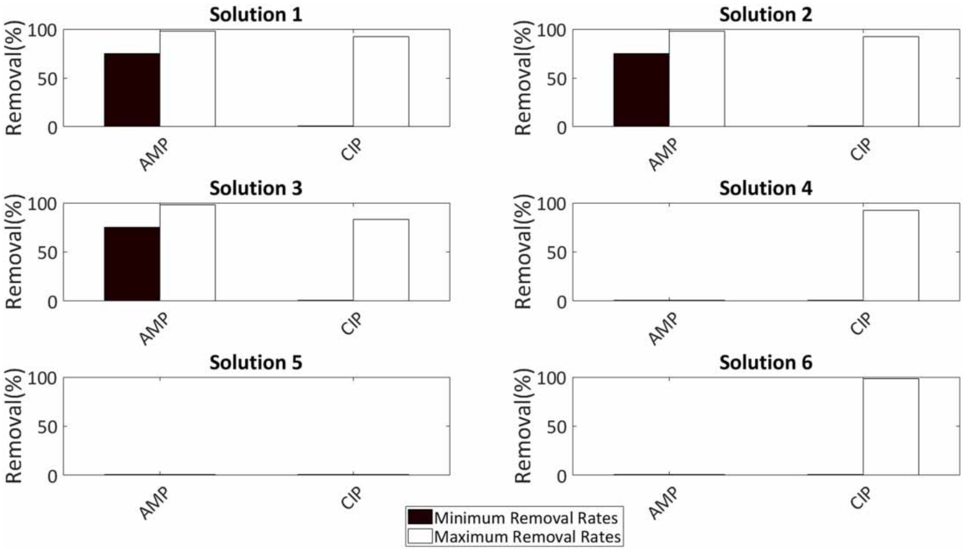

Figure 5 | Percentage of CECs removed from the different treatment solutions produced from WiSDOM-CEC for Delhi.

Table 5 | Wastewater treatment solutions taken from the WiSDOM tool for Karnataka

Solution number	Treatment train
1	Grit chamber → sedimentation → CASP + secondary sediment → ultrafiltration → reverse osmosis
2	Sedimentation → submerged aerated filter → ultrafiltration → nanofiltration
3	Constructed wetlands polishing → chlorine dioxide
4	Constructed wetlands polishing → ultrafiltration
5	Coarse screen → fine screen → sedimentation → trickling filter + secondary sedimentation → microfiltration
6	Grit chamber → DAF → CASP + secondary sedimentation → ultrafiltration

S1 outperformed the other solutions in regard to the removal of conventional pollutants, followed by S2, S6, S4, S5, and finally S3 (Figure 6). However, S3 and S5 were the worst in regard to BOD and COD, whereas all other solutions ranked in the lower scores. On the other hand, regarding the sustainability indicators, S5 performed the worst for all three constraints. S3 and S4 were the best in regard to land requirements; however, their scores for CAPEX and OPEX were also low. S1 and S2 ranked highly for all the MOO objectives. Therefore, the best solution that met all the requirements and was able to remove conventional pollutants was S1.

From Figure 7, it is clear that S1 and S6 were the two solutions which were capable of removing the majority of the CECs found in the influent. The main difference between these two solutions was the addition of reverse osmosis and the use of DAF instead of sedimentation in S6. S1 had higher removal rates for all the CECs and was able to remove CAF, BPA, and DEET to 100%. However, both S1 and S6 were only able to remove TCS from 24% to 26%, unlike S5 was able to remove this contaminant from 86% removal to 97% removal. On the other hand, S5 was unable to remove NPX and had lower removal rates for the hormone Estrone (EST). The solution best suited to the removal of CECs and the removal of conventional pollutants is S1.

Tamil Nadu

Results for Tamil Nadu from the WiSDOM tool populated six optimised treatment solutions which fit the original constraints entered into the tool (found in Table S1, Supplementary Information). Table 6 displays the treatment train selected for each solution generated.

S6 outperformed all the solutions in regard to the removal of conventional pollutants, with S2 having similar results, apart from a slightly higher result for turbidity (Figure 8). However, this was still low in comparison to

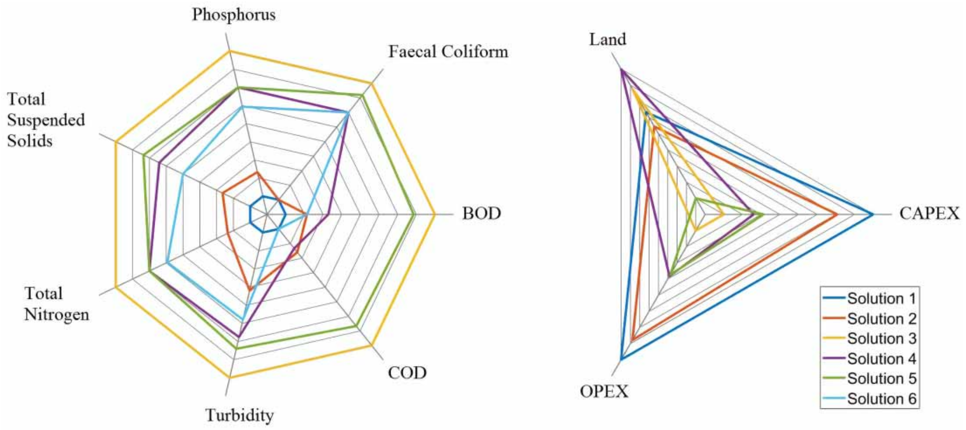

Figure 6 | Performance results from WiSDOM. (Left) Radar plot from the MOO optimisation for the results for the performance of the removal of conventional pollutants for all solutions. The higher the point on the axis the worse the solution has performed. (Right) Radar plot from WiSDOM from the MOO optimisation for the results for the performance of different sustainability indicator objectives (Land, OPEX, and CAPEX). The higher the point on the axis the better the solution has performed.

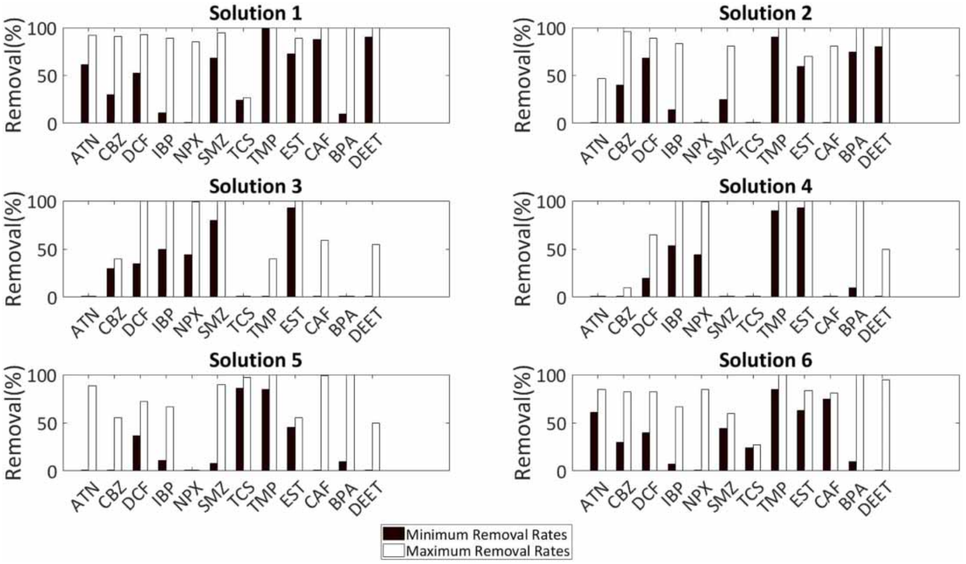

Figure 7 | Percentage of CECs removed from the different treatment solutions produced from WiSDOM-CEC for Karnataka.

S1, S3, and S4. S3 performed the worst having high values for all conventional pollutants, with S1 following close behind. S4 and S5 performed at the higher end of the scale, with S4 being slightly higher for all parameters. Regarding sustainability indicators S2, S5, and S6, all performed highly for CAPEX and OPEX with low-land requirement results. Whereas S3, S1, and S4 had a high-land requirement but low results for CAPEX and OPEX in the order listed. If land requirement is not as important as CAPEX and OPEX, then S4 would be an ideal solution in regard to meeting the removal of conventional pollutants. However, if CAPEX and OPEX are not important, then S6 or S2 would then be the best solution in removing conventional pollutants and meeting the requirements set as constraints in the WiSDOM tool.

Figure 9 displays the removal through each treatment train of each EC which was found in the influent in Tamil Nadu. S1 and S2 were the only solutions able to remove all the CECs; however, S1 had low removal rates for ERY, reaching only 15% removal, whereas S2 was able to

Table 6 | Wastewater treatment solutions taken from the WiSDOM tool for Tamil Nadu

Solution number	Treatment train
1	Constructed wetlands → advanced oxidation – UV/O_3
2	Grit chamber → sedimentation → activated sludge process + secondary sedimentation → microfiltration → nanofiltration
3	Constructed wetlands polishing → chlorine dioxide
4	Constructed wetlands polishing → ultrafiltration
5	Coarse screen → fine screen → sedimentation → trickling filter + secondary sedimentation → ultrafiltration
6	Grit chamber → sedimentation → trickling filter + secondary sedimentation → microfiltration → nanofiltration

remove 72% of this contaminant. S4 was an ideal solution for meeting the requirements set in the WiSDOM tool but was unable to remove ATN, ERY, SMZ, TCS, and CAF. Therefore, S4 is not an ideal solution when it comes to the main objective of removing CECs. S5 and S6 were unable to remove NPX and OPX, and for the other four solutions, removal rates were the same ranging from 44% removal to 99%. S1 would be the ideal solution to remove CECs and still was able to remove conventional pollutants to the required standards (Figure 8). However, the solution that fits all constraints to a better standard and was still able to remove CECs would be S2. This solution was able to remove all CECs and had a lower removal for Ofloxacin (OFC) of 45% and for TCS reaching a maximum removal of 27%.

Removing contaminants of emerging concern

CECs in the same category would be expected to behave in the same way due to having similar properties. However, each individual CEC has distinct physical and chemical properties resulting in a unique response to breaking down in unit processes or reacting to certain treatment options. The following section characterises the two different drug classes of pharmaceuticals (NSAIDs and antibiotics) and other categories explored in this study to determine if CECs in the same category have the same removal rates.

Antibiotics

In this study, both CIP and OFX were not detected in the same location; however, one can look at their removal through different unit processes. Across all sites, CIP was infectively removed through the use of CWs, trickling filters, ultrafiltration, or advanced oxidation, whereas the greatest removal rates were achieved for OFX. The addition of chlorine dioxide as a tertiary treatment removal saw close to 100% removal. Greater than 50% removal was also seen when primary and secondary sedimentation was used, alongside activated sludge processes or powdered activated carbon. OFX on the other hand showed little removal during these techniques. The same results are reflected in

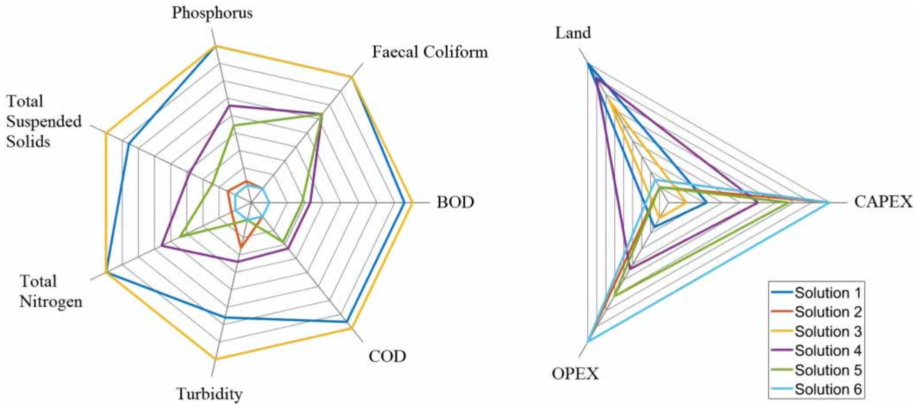

Figure 8 | Performance results from WiSDOM. (Left) Radar plot from the MOO optimisation for the results for the performance of the removal of conventional pollutants for all solutions. The higher the point on the axis the worse the solution has performed. (Right) Radar plot from WiSDOM from the MOO optimisation for the results for the performance of different sustainability indicator objectives (Land, OPEX, and CAPEX). The higher the point on the axis the better the solution has performed.

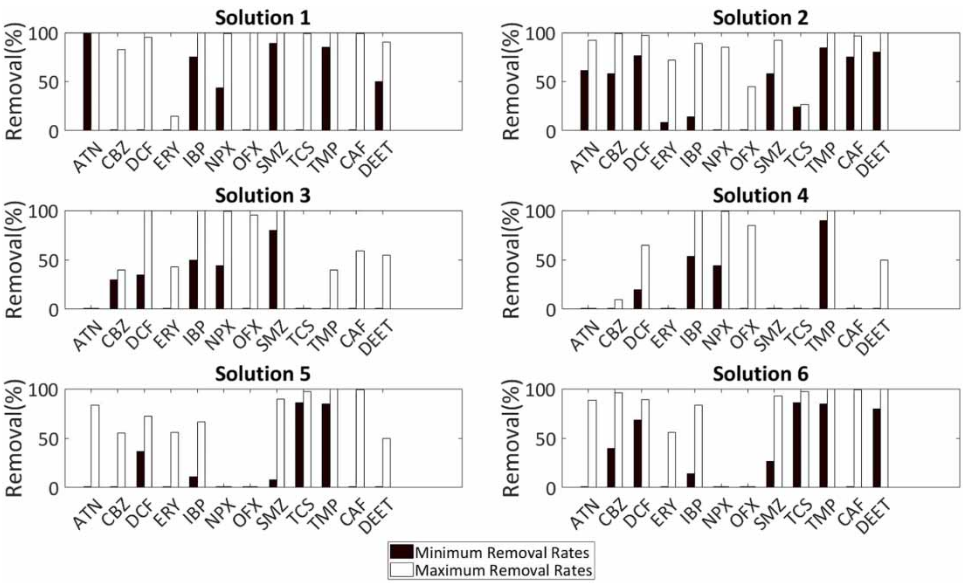

Figure 9 | Percentage of CECs removed from the different treatment solutions produced from WiSDOM-CEC for Tamil Nadu.

a study by Michael *et al.* (2013) who found that the best removal for OFX used advanced oxidation techniques which led to 83% removal and up to 85% removal was achieved through the use of CWs. The study also supported the removal of CIP showing higher removal rates from primary sedimentation (78%), secondary sedimentation (83%), and powdered activated carbon (100%). On the other hand, a study by Jia *et al.* (2012) found similar removal rates between the two fluoroquinolones through a sewage treatment plant with an overall removal of 64% for CIP and 66% for OFL (Jia *et al.* 2012), although a lower initial concentration of CIP was detected in the raw sewage.

Nonsteroidal anti-inflammatory drugs

DCF, IBP, and NPX are all classed as anti-inflammatory substances. In the case of Uttar Pradesh, the three substances exhibited similar removal rates exceeding 90% for solutions involving CWs as a unit process, combined with advanced oxidation or chlorine dioxide. The levels of DCF dropped to below 70% removal when ultrafiltration was combined with CWs. DCF and IBP had similar removal rates when sedimentation and trickling filters were used; however, NPX was not removed during this process. All three contaminants were removed between 50% and 80% when activated sludge was combined with sedimentation and ultrafiltration. These low removal rates for activated sludge are not reflected in recent studies in the literature where NPX had a 94–99% removal efficiency, IBP was removed to 99%, and DCF had the lowest removal rate from 92% to 98%. Similarly, DCF had low removal rates of 77–98% for tertiary treatment, and 9–21% for primary treatment, NPX followed with 91–98% and 17–55%, respectively. IBP had a higher minimal removal rate recorded for the primary treatment of 25%; however, the maximum removal only reached 53% (Larsson *et al.* 2014). 100% removal was achieved for tertiary treatment as displayed in the solutions for Uttar Pradesh. In Karnataka, NPX was not removed when sedimentation, trickling filters, and other filtration techniques were used; otherwise, the three contaminants displayed similar removal efficiencies within 10% of each other. This was also the case for the other solutions when alike unit processes were used as previously mentioned. In the literature, varying removal rates exist for each NSAID, suggesting that other controlling factors might be present as the studies were carried out in different locations. For NPX, varying removal rates have been found for different experiments where Snyder *et al.* (2007) found a removal via PAC of 50%; however, Nam *et al.* (2014) found a removal efficiency of 95% (Nam *et al.* 2014; Snyder *et al.* 2007). CWs seemed a prominent treatment option for removing NSAIDs, suggested by a greater than 90% removal in this study. However, Luo *et al.* (2014) found a removal from 44% to 99% for NPX, 40% for IBP, and 50% for DCF, although when used as a final treatment option such as a polishing pond, the removal increased to greater than 90%.

Removal of hormones, stimulants, personal care products, and insect repellents

EST, found in Karnataka, was able to be removed via the unit processes outputted in the WiSDOM tool. CWs and advanced oxidation are a successful treatment solution for this hormone, shown in S1, S3, and S4 in Figure 7. These solutions have removal rates of 100% and 98%, respectively, in comparison to 26% to 75% removal available with the use of sedimentation, CASP, and filtration methods.

High concentrations of CAF were found across the South, West, and Central regions of India, with concentrations reaching 220,000 ng/L (Table 2). With high concentrations being found in these regions, it is important to produce a treatment solution effective at removing the contaminant. Many studies have been carried out on the removal of CAF through wastewater treatment plants, proving that effective solutions should incorporate the following unit processes. Sedimentation is able to remove around 81% and this proved to be the main removal process along with reverse osmosis which was able to remove 50–80% (Luo *et al.* 2014). Many studies which have been carried out have focused on the removal throughout the whole treatment train and not the removal through individual unit processes (Sui *et al.* 2010; Froehner *et al.* 2011).

Two personal care products, BEN and BPA, were found in the influent wastewater of Nagpur and Karnataka, respectively. The treatment trains that were ideal to the area of Nagpur in regard to the MOO objectives were not suited to removing BEN (Figure S3 – 4, Supplementary Information). BEN is described as one of the most common UV filters with endocrine-disrupting effects; therefore, it is important to determine a unit process able to remove this compound. Most of the existing published literature has found that removal varied from 40% to 100%, with the use of advanced oxidation (Zúñiga-Benítez *et al.* 2016). This substance has high lipophilic properties; therefore, further investigations should be carried out on unit processes where sorption onto solids or biodegradation occurs (Gong *et al.* 2015). On the other hand, BPA was able to be removed during five of the chosen treatment trains in Karnataka with submerged-aerated filters able to remove up to 95% of the contaminant. Zielińska *et al.* (2016) found that BPA is difficult to remove during conventional biological methods, but found microfiltration and NF to have positive removal rates leading to 100% removal (Zielińska *et al.* 2016). However, other research has found lower removal rates for these unit processes reaching up to only 10% (Zhu & Li 2013).

The highest influent concentration recorded for DEET was found in Karnataka with a concentration of 388 ng/L and the lowest recorded concentration was 4 ng/L in Bihar. High removal rates were found for DEET and most of the treatment solutions produced were able to remove up to 90% of DEET, with NF and ultrafiltration able to remove 50–100% (Sui *et al.* 2010).

The treatment train solutions created from the WiSDOM tool for each region in India were effectively produced to suit the original constraints entered into the tool. These solutions showed the ability to remove conventional pollutants in order to allow for water reuse application in India. The chosen treatment trains were also able to remove the CECs found in the influent; however, in some cases, removal via other treatment options would be more suited, such as for BEN, where no treatment train chosen was able to remove the contaminants. However, in some cases, CECs in the same categories exhibited similar removal rates across treatment solutions; in most cases, each CEC exhibited different removal rates. When compared to other studies, no two CECs in a category or drug class (e.g., NSAIDs) display the same properties or exact removal efficiencies. This is because each contaminant, whether hydrophilic or hydrophobic, displays individual physical, chemical, and biological characteristics resulting in an individual breakdown of the pollutant.

In terms of the highest recorded concentration across India, CAF was effectively removed during sedimentation and advanced oxidation treatment options; however, for other CECs, this was not an effective removal technique. Advanced oxidation techniques and the use of reverse osmosis, although practical and efficient, are not suited to rural areas due to the cost associated with this treatment method, both CAPEX and OPEX. CWs were effective at removing the majority of recorded emerging contaminants and are a sustainable, cost-effective solution. However, in some locations of India where land requirement is a restriction, such as urban areas, this is not a feasible solution resulting in the selection of other unit processes.

Future applications

Currently, this research focuses on determining effective solutions for the removal of CECs in developing countries such as India. This is because, for most developed countries, the infrastructure is already in place for wastewater treatment and it would be costly to recreate treatment train solutions for application. However, a decision support tool could be developed that analyses the existing treatment unit processes and provides an additional unit process that could be implemented to achieve the required results. Additionally, the focus was applied to developing countries as the decision support tool WiSDOM was originally created to generate water reuse solutions in India. Therefore, data were collected on emerging contaminants in India. Since the information included in the technology library is not case-specific, future application could involve applying the tool to calculate the removal of CECs in developed countries.

To further this work, the functionality of the add-on worksheet can be integrated directly into WiSDOM by expanding the source code. Additionally, the ESP removal model can be incorporated directly into WiSDOM by imposing a limited number of CECs as constraints (based on the user's preference) in addition to the conventional contaminants. This will allow the tool to decide on best solutions by also incorporating the removal of the chosen CECs selected by the user. Furthermore, as the ESP can be easily altered to suit a different developing country if data are available regarding the removal of CECs. This could then be combined with different decision support tools that currently do not incorporate the removal of CECs.

CONCLUSIONS

The aim of this study was to determine the effectiveness of a decision support tool for producing optimal wastewater management solutions for developing countries. This was done by using an existing decision support tool for India, WiSDOM, and building an ESP that works alongside the tool, taking the treatment train solutions from WiSDOM and using these to calculate the removal of CECs through the unit processes. Different regions of India were analysed to show varying constraints and input data. With CECs becoming an increasing cause of concern, the ESP was designed to calculate the minimal and maximum removal of CECs through the produced treatment solutions. Natural processes, such as CWs, are the most effective at removing CECs along with being a more sustainable solution. However, due to the constraints such as land requirements along with cost, these are not always the best solution as shown by the low incidence of this unit process being chosen in the WiSDOM tool. Although CECs classed under the same category have similar physical, chemical, and biological parameters, these contaminants are not always removed in the same way. For example, the pharmaceutical group NSAIDs which showed different removal rates between DCF, IBP, and NPX when passed through the same treatment solution. This can be seen in Uttar Pradesh, Karnataka, Tamil Nadu, and Bihar (in S3 in the Supplementary Information). In Tamil Nadu, removal rates ranged from 0% to 95% for DCF, 75% to 100% for IBP, and 44% to 99% for NPX for the first solution (CWs, advanced oxidation, and UV/O_3). In S5 (coarse screen, fine screen, sedimentation, trickling filter and secondary sedimentation, and ultrafiltration), the removal rates showed a greater difference with removal rates ranging from 36.8% to 72% for DCF, 10.7% to 66.5% for IBP, and 0% for NPX. This demonstrates that although it is expected that CECs under the same class of pharmaceutical or personal care product, for example, should be removed in the same way, this is not always the case as each substance has its own properties.

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SUPPLEMENTARY MATERIAL

The Supplementary Material for this paper is available online at https://dx.doi.org/10.2166/hydro.2019.031.

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